1-Cyclohexene-1-carboxylic acid, 4-(1,5-dimethyl-3-oxohexyl)-, methyl ester, [R-(R*,R*)]-

Other names: 1-Cyclohexene-1-carboxylic acid, 4-(1,5-dimethyl-3-oxohexyl)-, methyl ester, (1R,4R)-(+)-
(+)-Juvabione
Juvabione
Juvabionine

Inchi: InChI=1S/C16H26O3/c1-11(2)9-15(17)10-12(3)13-5-7-14(8-6-13)16(18)19-4/h7,11-13H,5

InchiKey: IIWNDLDEVPJIBT-UHFFFAOYSA-N

Formula: C16H26O3

SMILES: COC(=O)C1=CCC(C(C)CC(=O)CC(C)C)CC1

Mol. weight [g/mol]: 266.38

CAS: 17904-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-239.10	kJ/mol	Joback Method
hf	-640.88	kJ/mol	Joback Method
hfus	27.20	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.527		Crippen Method
mcvol	230.150	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	718.45	K	Joback Method
tc	923.93	K	Joback Method
tf	382.83	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.69	J/mol×K	718.45	Joback Method
cpg	755.42	J/mol×K	889.68	Joback Method
cpg	741.49	J/mol×K	855.44	Joback Method

cpg	726.48	J/mol×K	821.19	Joback Method
cpg	710.36	J/mol×K	786.94	Joback Method
cpg	693.10	J/mol×K	752.70	Joback Method
cpg	768.27	J/mol×K	923.93	Joback Method
dvisc	0.0001141	Pa×s	718.45	Joback Method
dvisc	0.0001528	Pa×s	662.51	Joback Method
dvisc	0.0002160	Pa×s	606.58	Joback Method
dvisc	0.0003274	Pa×s	550.64	Joback Method
dvisc	0.0005453	Pa×s	494.70	Joback Method
dvisc	0.0010344	Pa×s	438.77	Joback Method
dvisc	0.0023659	Pa×s	382.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17904277&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume